ECOLE NORMALE SUPERIEURE

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April 1998

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Abstract

Let a circuit C of length n be the boundary of a disc such that C has k vertices of valency 3 and other $n-k$ vertices of valency 2. We relate to C a sequence $a(C)=a_1,...,a_k$ such that $n=k+\sum_1^k a_i$ and a_i is the number of vertices of valency 2 between i-th and $(i+1)$-th vertices of valency 3. We study hexagonal sequences $a=a_1a_2...a_k$ determining a partition of the disk into hexagons and enumerate all hexagonal sequences without zeros. We give some applications to fullerenes. .

1 Introduction

In [DeGr97a], [DeGr97b], one considers planar cubic maps p_n, $p=3,4,5$, having n vertices and only p-gonal and hexagonal faces. These graphs are the 1-skeletons of polyhedra p_n. The Euler relation implies that the number s_p of p-faces is the same for graphs p_n, namely, s_3=8, s_4=6, s_5=12. The minimal graphs p_n have no hexagonal faces, and are skeletons of 3_8= octahedron, 4_6= cube, 5_{12}= dodecahedron.

There are problems of enumerations of graphs p_n having fixed configurations of q-faces, in particular, problem of existence of such graphs. In this note we give an algorithm of construction of some such graphs without drawing them explicitly.

For this purpose, we consider one-connected *polygonal systems*, i.e. simple graphs consisting of polygons such that the intersection of any two polygons are either empty or consist of one edge. It means that the inner vertices have valency 3 and the boundary vertices have valency 2 or 3. These graphs (or maps) are considered in Organic, Physical and Mathematical Chemistry.

We are interested especially in *hexagonal systems* which consist only of hexagons. Sometimes these systems are called *benzenoid systems* or *benzenoid graphs*. We relate to the boundary circuit C of length n a sequence $a(C)=a_1...a_k$ such that $n=k+\sum_1^k a_i$, where k is the number of vertices of valency 3 and a_i is the number of vertices of valency 2 between i-th and $(i+1)$-th vertices of valency 3. We call the sequence $a(C)$ *hexagonal* if C

*This work was supported by Volkswagen-Stiftung (RiP-program at Oberwolfach).

is the boundary of a hexagonal system. The aim of the paper is to characterize hexagonal sequences.

It seems to us that the method of sequences may be useful in any algorithm enumerating maps p_n. Similar sequences are used in a fast algorithm of [BDPS97] enumerating fullerenes 5_n. The task of filling the disc inside the circuit C by a planar graph which is a part of the map 5_n and has C as the boundary circuit is called in [BDPS97] *PentHex Puzzle*.

2 Boundary circuits of a map

Consider a simple cubic planar map, i.e. lying on a plane cubic plane graph. Call its minimal circuits *faces*. A p-gonal face (p-face or p-gon) is face with p vertices (and p edges). We consider maps $\mathcal{M}_p$ having many mutually adjacent hexagonal and s_p p-gonal faces, for fixed p, $2 \le p \le 5$.

Consider a simple, i.e. non self-intersecting, circuit C of $\mathcal{M}_p$. We call C *boundary circuit*. Since $\mathcal{M}_p$ is planar, C has naturally the inner domain $D(C)$ and the outer domain $\overline{D}(C)$. Since $\mathcal{M}_p$ is cubic, each vertex of C is incident to exactly one edge not belonging to C.

Call by *tail* any edge of $\mathcal{M}_p$ incident to exactly one vertex of C. Let C has k tails t_i, $1 \le i \le k$, lying in the inner domain $D(C)$. We relate to C the sequence $a(C) = a_1 a_2 ... a_k$, where a_i is the number of vertices of C lying between t_i and t_{i+1}. (The tails incident to these a_i vertices lie in the outer domain $\overline{D}(C)$). The number k is called the *length* $l(a)$ of the sequence $a(C)$. The sequence $a(C)$ is considered up to reversing and a cyclic shift, i.e. the sequences $a^{q\pm} \equiv a_{q\pm1} a_{q\pm2} ... a_{q\pm k}$, $q = 0, 1 ...$, (all indices with equal signs) are considered as identical. If a is obtained from a' by a shifting and reversion, we write $a \sim a'$. The indices of the sequences are taken modulo k. If C has n vertices, then $k + \sum_1^k a_i = n$.

The difference

$$\lambda(a) \equiv \lambda(C) = \sum_1^k a_i - k = \sum_1^{l(a)} a_i - l(a) \qquad (1)$$

is called *leftness* of C in [GrZa74]. (Unfortunately the name *leftness* shows on an orientation of C).

Similarly, the $\overline{k}$ tails s_i, $1 \le i \le \overline{k}$, lying in the outer domain $\overline{D}(C)$, determine the sequence $\overline{a}(C) = \overline{a}_1 \overline{a}_2 ... \overline{a}_{\overline{k}}$ of length $l(\overline{a}) = \overline{k}$. Obviously, $\overline{k} = n - k = \sum_1^k a_i$ and $\sum_1^{\overline{k}} \overline{a}_i = k = n - \overline{k}$. Call the sequence $\overline{a}(C)$ the *complement* of $a(C)$. Similarly, $a(C)$ is the complement of $\overline{a}(C)$. Since $l(\overline{a}) = \overline{k} = \sum_1^k a_i$, we have

$$\lambda(a) = l(\overline{a}) - l(a) = -\lambda(\overline{a}). \qquad (2)$$

The correspondence between $a(C)$ and $\overline{a}(C)$ is given by the following correspondence of subsequences of $a(C)$ and $\overline{a}(C)$. If C is the boundary of an n-face $D(C)$, then $a(C)$ is empty and $\overline{a}(C) = 00...0$ consists of n zeros. If $a(C) = 1...1$, then $\overline{a}(C) = a(C)$. Otherwise, for $x > 1$, $y > 1$ and $p \ge 0$, we have

$$x1^p y \Longleftrightarrow 0^{x-1} 1^{p+1} 0^{y-1},$$

$$x1^p0^{y-1} \Longleftrightarrow 0^{x-1}1^py,$$

where we use denotation i^p for $\underbrace{i...i}_{p}$. If $p = 0$, then the corresponding sequence is empty. Here subsequences of consecutive zeros and ones are maximal. Recall that sequences $a(C)$ and $\overline{a}(C)$ are considered cyclically. Hence there are k neighboring pairs a_ia_{i+1} in a sequence of length k. As an example of applying above correspondence, we have $\overline{44} = 00010001$, $\overline{333} = 001001001$, and $\overline{120310} = 1020012$.

If all faces of $\mathcal{M}_p$, lying in the inner domain of C and adjacent to C, are p-gons, $2 \leq p \leq 6$, then we have

$$0 \leq a_i \leq 4, \text{ for all } i. \tag{3}$$

For $0 \leq l \leq 4$, let n_l be the number of i with $a_i = l$. Then

$$\lambda(a) = 3n_4 + 2n_3 + n_2 - n_0. \tag{4}$$

Call a sequence a *balanced* if $\lambda(a) = 0$. The equality (2) shows that the complement of a balanced sequence is also balanced. Call a sequence a *Petrie* if it consists only of ones, i.e. $a = 1^k$ for some $k > 0$. The corresponding circuit $C(a)$ is called *Petrie circuit*. The equality (4) shows that a Petrie sequence is balanced.

A condition for leftness $\lambda(a)$ of a sequence a can be obtained from the Euler relation. We consider more general case. Suppose that a planar map $\mathcal{M}_p$ has mutually non-intersecting boundary circuits C_i, $1 \leq i \leq q$, which are faces of $\mathcal{M}_p$. Let all other faces of $\mathcal{M}_p$ be hexagonal or p-gonal for fixed p, $2 \leq p \leq 5$. The vertices of C_i have valency 2 or 3. Let v_2 and v_3 be the numbers of all vertices of all C_i of valency 2 and 3, respectively. We denote $v_2 - v_3 = \lambda(C_1, ..., C_q)$.

Lemma 1 *Let q be the number of the circuits C_i and s be the number of p-faces. Then $\lambda(C_1, ..., C_q) = ps - 6(q + s - 2)$.*

Proof. We use the Euler relation $v - e + f = 2$, where v, e and f are the numbers of vertices, edges and faces of $\mathcal{M}_p$. We have

$v = v_2 + v_3 + x$,

$2e = 2v_2 + 3(v_3 + x)$,

$sp + 6h = v_2 + 2v_3 + 3x = v_2 - v_3 + 3(v_3 + x)$,

where x is the number of vertices of $\mathcal{M}_p$ belonging to no C_i, and h is the number of hexagonal faces of $\mathcal{M}_p$. Hence $f = s + h + q$. Substituting these values in the Euler relation, we obtain the asserted equality.

If $q = 1$, we suppose that all hexagons and p-gons lie in the inner domain $D(C)$ of the boundary circuit $C = C_1$. Lemma 1 gives $\lambda(C) = 6 - s(6 - p)$. Consider the sequence $a(C) = a_1...a_k$. Obviously, $k = v_3$ and $v_2 = \sum_1^k a_i$. Hence, for the sequence $a = a(C)$, we have

$$\lambda(a) = 6 - s(6 - p). \tag{5}$$

Since $p \leq 6$, we have $\lambda(a) \leq 6$, and $\lambda(a) = 6$ if $s = 0$.

Suppose, we have a sequence a with leftness $\lambda(a)$. Then there is a boundary circuit $C(a)$ surrounding a disc partitioned into p-gons and hexagons if and only if the amount

$$s(a) = \frac{6 - \lambda(a)}{6 - p} \tag{6}$$

is an integer. In this case, $s(a)$ is the number of p-gons surrounded by $C(a)$. In particular, if $\lambda(a) = 6$, $C(a)$ surrounds only hexagons. This means that all p-gons lie in the outer domain $\overline{D}(C)$. Recall that $\overline{a}$ is the sequence corresponding to the boundary circuit of $\overline{D}(C)$. By (4), $\lambda(\overline{a}) = -6$, and $s(\overline{a}) = s_p \equiv \frac{12}{6-p}$, the number of p-gons in any map $\mathcal{M}_p$.

Let a be balanced, i.e. $\lambda(a) = 0$. Then $s(a) = \frac{6}{6-p} = \frac{1}{2}s_p$. Hence we have

Lemma 2 *If a sequence a is balanced, then the corresponding simple circuit $C(a)$ partitions any map $\mathcal{M}_p$ into two domains each containing a half of all p-gons.*

Obviously, a minimal sequence $a(C)$ corresponds to the boundary of a p-gon, that has no tails in $D(C)$, and therefore $a(C)$ is empty. A minimal non-empty sequence $a(C) = p-2, p-2$ corresponds to the boundary of two adjacent p-gons.

There are 5^k abstract sequences a of length k satisfying (3). Obviously, we can relate a circuit $C(a)$ to each of such sequences. If a has length k, then $C(a)$ has $k + \sum_1^k a_i$ vertices and k tails. Denote by $D(a)$ the disc boundary of which is $C(a)$.

Let a sequence $a = a(C)$ corresponds to the boundary circuit C of a map $M(a)$. Recall that there are $a_i + 1$ edges of C between the tails t_i and t_{i+1}. These $a_i + 1$ edges are common edges of C and a p-gon or a hexagon. Denote it by h_i.

Suppose that h_i has no other edges common with C. We connect the tails t_i and t_{i+1} in an arc. This arc is the boundary circuit of a p-gon (or a hexagon) h_i and it may be a p-gon if $a_i \le p-2$. Suppose that $a_i = p-2$. Then h_i has $p-1$ edges common with C. The p-th edge connects two vertices of C, namely, the end-vertices of the tails t_i and t_{i+1}. This edge is also an edge of two coinciding p-gons $h_{i-1} = h_{i+1}$. If $a(C)$ has an element $a_i = p-3$, then h_i has $p-2$ edges common with C, and two other edges of h_i are edges of h_{i-1} and h_{i+1}. Hence the p- and p'-gons h_{i-1} and h_{i+1} have a common edge that is incident to a vertex of h_i.

Connect the neighboring tails t_i and t_{i+1} for to form the p-gon h_i. Consider the new circuit C' that is the boundary of $D(C)$ without the p-gon h_i. Then we obtain the new sequence

$$a(C') = f_p(a_1 ... \hat{a}_i ... a_k).$$

Here the operation f_p transforms $a(C)$ such that the triple $a_{i-1}a_i a_{i+1}$ (that we denote as the triple acb) is changed in accordance with a value of c, $0 \le c \le 4$, as follows

$$f_p(a\hat{c}b) = \begin{cases} a+1, 0^{p-3-c}, b+1 & \text{if } c \le p-3 \\ a+b+2 & \text{if } c = p-2. \end{cases} \tag{7}$$

If $acb = a_{i-1}a_i a_{i+1}$, we say that the operation f_p is *applied to a with respect to a_i* and *closes* the hexagon h_i.

Recall that f_p may by applied to close h_i if the only edges of h_i common with C are the $a_i + 1$ edges between t_i and t_{i+1}.

Note that f_p increases, decreases or does not change the length of $a(C)$. If $a_i \leq 2$ for all i, then the operations f_6 do not reduce length of a. Call such a sequence *irreducible.* According to (4), the leftness of an irreducible sequence a is equal to

$$\lambda(a) = n_2 - n_0.$$

Recall that Petrie sequences are irreducible.

3 Hexagonal sequences

Call a sequence $a = a_1 a_2 ... a_k$ *hexagonal* if it corresponds to a circuit surrounding a partition of the disc $D(a)$ into hexagons. Let $h(a)$ be the number of hexagons in this partition. Note that $h(44) = 2$, $h(333) = 3$. Obviously, a hexagonal sequence satisfies (3). But most of sequences satisfying (3) are not hexagonal.

Since $s = 0$ in (5) for a hexagonal sequence a, we have

Corollary 1 *All hexagonal sequences a have the same leftness $\lambda(a) = 6$.*

Corollary 1 and (2) imply that the complement of a hexagonal sequence is not hexagonal. For example, a balanced and, in particular, Petrie sequence is not hexagonal.

Now we describe an algorithm **A** recognizing hexagonal sequences. Suppose that a sequence a is hexagonal, i.e. it corresponds to a partition $P(a)$ of the disc $D(a)$ with the boundary circuit $C = C(a)$. Let $M(a)$ be the graph (map) of $P(a)$. Denote by v_i the vertex of the tail t_i common with C. Recall that $a_i + 1$ edges of C between t_i and t_{i+1} are edges of the hexagon h_i. The recognition algorithm **A** uses several reductions of the sequence a to a sequence of less length.

The difficulty of recognition of hexagonal sequences is that some hexagons h_i and h_j for $|i - j| \geq 2$ can coincide or have common edges. However if $a_i = 4$ or 3, then h_i has common edges only with $h_{i\pm1}$, but h_{i-1} and h_{i+1} coincide or have a common edge, respectively. This means that we can always apply the operation f with respect to $a_i = 4$ or 3 for to close h_i.

In order to find hexagons h_i and h_j with $|i - j| \geq 2$ coinciding or having a common edge, we proceed as follows. Consider a shortest path p_{ij} between vertices v_i and v_j in the map $M(a)$. The length $l(p_{ij})$ of the path is the number of its edges. If $l(p_{ij}) = 1$, then the hexagons h_{i-1} and h_j coincide, as well as the hexagons h_i and h_{j-1}. If $l(p_{ij}) = 2$, then there are two cases: either h_{i-1} and h_j coincide or they have a common edge. Then h_i and h_{j-1} either have a common edge or coincide, respectively. If $l(p_{ij}) = 3$, then h_{i-1} and h_j as well as h_i and h_{j-1} have a common edge. There are also two cases: h_{i-1} and h_{j-1} have either one or two common edges with p_{ij}. Then, respectively, h_i and h_j have two and one common edges with p_{ij}.

The vertices v_i and v_j partition the circuit C into two connected components C' and C''. These components are related to two subsequences of a that we denote by $a_j a' a_{i-1}$ and $a_i a'' a_{j-1}$. The path p_{ij} partitions the disc $D(a)$ into two domains with the boundaries $C^+ = C' \cup p_{ij}$ and $C^- = C'' \cup p_{ij}$. Denote the sequences corresponding to $C^\pm$ by $g_{ij}^{\pm l}(a)$, where $l = l(p_{ij})$. Call the transformation of a into the two sequences $g_{ij}^{+l}(a)$ and $g_{ij}^{-l}(a)$ the *reduction* g_{ij}^l.

It is easy to verify that

$$g_{ij}^{+1}(a) = a', a_{i-1} + a_j + 2 \text{ and } g_{ij}^{-1}(a) = a'', a_{j-1} + a_i + 2,$$

$$g_{ij}^{+2}(a) = a', a_{i-1} + a_j + 3 \text{ and } g_{ij}^{-2}(a) = a'', a_{j-1} + 1, a_i + 1,$$

$$g_{ij}^{+3}(a) = a', a_{i-1} + 1, a_j + 2 \text{ and } g_{ij}^{-3}(a) = a'', a_{j-1} + 1, a_i + 2,$$

For $l = l(p_{ij}) = 2$ and 3, we give the sequences of the first case. The sequences of the second case are obtained by the transposition of the indices i and j.

Suppose that a is irreducible. Then for the sequences $g_{ij}^{\pm l}(a)$ satisfy (3), it is necessary that

$$a_{i-1} + a_j \leq 2, \quad a_{j-1} + a_i \leq 2, \qquad \text{for } l = 1, \qquad a_{i-1} + a_j \leq 1, \quad \text{for } l = 2. \tag{8}$$

For the sequences $g_{ij}^{\pm l}(a)$ be hexagonal, it is necessary that they have leftness equal to 6. Let the subsequences $a_j a' a_{i-1}$ and $a_i a' a_{j-1}$ have n_2', n_2'' twos and n_0', n_0'' zeros, respectively. Then, for example, $\lambda(a_j a' a_{i-1}) = n_2' - n_0'$. Note that $l(g_{ij}^{+1}(a)) = l(a_j a' a_{i-1}) - 1$. Hence, according to (1), $\lambda(g_{ij}^{+1}(a)) = \lambda(a_j a' a_{i-1}) + l(a_j a' a_{i-1}) + 2 - l(g_{ij}^{+1}(a)) = \lambda(a_j a' a_{i-1}) + 3$. Similarly, $\lambda(g_{ij}^{-1}(a)) = \lambda(a_i a'' a_{j-1}) + 3$. The same equalities hold for $g_{ij}^{\pm 3}(a)$. Repeating considerations for $l = 2$, we obtain that the necessary condition for hexagonality of $g_{ij}^{\pm l}(a)$, $l = 1, 2, 3$, is validity of the following equalities:

$$n_2' - n_0' = n_2'' - n_0'' = 3, \quad \text{for } l = 1, 3, \quad n_2' - n_0' = 2, \quad n_2'' - n_0'' = 4, \text{ for } l = 2. \tag{9}$$

Obviously, if, for given l, both the sequences $g_{ij}^{\pm l}(a)$ are hexagonal, then the sequence a is also hexagonal. Suppose that the sequences $g_{ij}^{\pm l}(a)$, $1 \leq l \leq 3$, are not hexagonal. Then if a is hexagonal, the hexagons h_{i-1} and h_j similarly as h_i and h_{j-1} have no common edges. If it is true for all pairs ij, then C can be considered as the boundary of a ring $R = R(a)$ of k hexagons h_i, $1 \leq i \leq k$ such that two hexagons h_i and h_j of R are adjacent if and only if either $j = i + 1$ and the adjacency edge is t_i or $j = i - 1$ and the adjacency edge is t_{i-1}.

The circuit C is the outer boundary of R. Let C^* be the inner boundary of R. We can consider the tails t_i of C as tails of C^*, too, and code C^* by the sequence

$$a(C^*) = a_1^*, ..., a_k^*,$$

where $a_i^* = 2 - a_i$. In fact, the hexagon h_i has $a_i + 2$ vertices on C and $a_i^* + 2$ vertices on C^*. Hence $(a_i + 2) + (a_i^* + 2) = 6$, i.e. $a_i + a_i^* = 2$. We call the sequence $a(C^*)$ *dual* of the sequence a and denote it by a^*. Using the definition, we see that

$$\lambda(a^*) = -\lambda(a). \tag{10}$$

Note that if a is a Petrie sequence, then $a^* = a$ is also Petrie and $\lambda(a) = 0$.

Obviously if the sequence $\overline{a^*}$ is hexagonal, then it determines a partition of the disc $D(a) - R(a) = D(\overline{a^*})$. According to (2) and (10), $l(\overline{a^*}) = l(a) + \lambda(a^*) = l(a) - \lambda(a) = l(a) - 6$. Hence the transformation of a into $\overline{a^*}$ reduces length of the sequence.

The reduction algorithm **A** is as follows. If a is not irreducible, apply the operation $f \equiv f_6$ with respect to $a_i = 4$ and 3 until a will be either 44 (and then a is hexagonal) or irreducible. In the last case use the reduction $a \to \overline{a^*}$, and apply **A** to $\overline{a^*}$. If $\overline{a^*}$ is not hexagonal, then for all pairs ij satisfying (8) and (9), for $l = 1, 2, 3$, apply reductions g^l_{ij}, and then apply the algorithm **A** to the reduced sequences $g^{\pm l}_{ij}(a)$.

Note, if a is hexagonal, then either $\overline{a^*}$ is hexagonal or $g^{\pm l}_{ij}(a)$ is hexagonal for at least one l and one pair ij. This proves that **A** recognizes hexagonality of a.

Remark. Suppose that a is irreducible and the reductions g^1_{ij} do not work for all pairs ij. Then the boundary circuit $C(a)$ is the boundary circuit of a ring R of hexagons. It seems that we can apply the reduction $a \to \overline{a^*}$. But the outer boundary circuit C^* of R can be self-intersecting by edges. In this case the sequence $\overline{a^*}$ is not hexagonal. This is why we have to introduce the reductions g^l_{ij} for $l = 2, 3$.

We are thankful to Mikhail Shtogrin for an example of a hexagonal sequence, where the reduction $a \to \overline{a^*}$ does not work. His example is the case $p = 5$ of the sequence $12^4 112^p 112^4 10^{p+2}$, $p \geq 0$. This sequence corresponds to a hexagonal system that cannot be embedded into the hexagonal lattice of regular hexagons lying on a plane.

4 Hexagonal sequences without zeros

Consider a hexagonal sequence consisting of regular hexagons of sidelength 1. Call a hexagonal system *convex* if the straight line connecting centers of any two its hexagons lies strictly inside the domain filled by hexagons. Hexagonal sequences without zeros correspond to convex hexagonal systems.

The task of reconstruction of a convex hexagonal system by its sequence can be called *convex Hex Puzzle*, since it is a special case of *convex PentHex Puzzle* of [BDPS97] without pentagons. We shall see below that this task has a unique well described solution.

The convex hull of centers of all hexagons of a convex hexagonal system is a (nonregular) hexagon H with parallel opposite sides. Sidelengths of H are equal to $\sqrt{3}p_i$, where $\sqrt{3}$ is distance between centers of two adjacent hexagons, and p_i is an non-negative integer, $1 \leq i \leq 6$. The hexagon H is generated if $p_i = 0$ for some i. If we prolong the sides 1, 3 and 5 until they intersect, then the intersection points are vertices of an equilateral triangle T, in which H inscribed. Sidelength of T is equal to

$$p = p_1 + p_2 + p_3 = p_3 + p_4 + p_5 = p_5 + p_6 + p_1. \tag{11}$$

These equalities show that H is determined by four independent parameters, for example, by p_1, p_3, p_5 and p.

(Cf. the description of triangulations of such a hexagon in [Th98]. The hexagon is represented as a large triangle of sidelength n minus three equilateral triangles that fit inside it of sidelengths q_1, q_2, q_3. These four parameters naturally satisfy the 7 inequalities: $n \geq 0$, $q_i \geq 0$, $q_i + q_j \leq n$, $i \neq j$, $i, j \in \{1, 2, 3\}$.)

If we prolong the even sides 2, 4, 6, then we obtain another equilateral triangle with another sidelength $p_2 + p_3 + p_4 = p_4 + p_5 + p_6 = p_6 + p_1 + p_2$.

It is easy to verify that the hexagonal sequence corresponding to a convex hexagonal system has no zero. If $p_i \geq 1$ for all i, then it has form

$$21^{p_1-1}21^{p_2-1}21^{p_3-1}21^{p_4-1}21^{p_5-1}21^{p_6-1}.$$

If $p_i = 0$ for one, two or three i, then the multiple 3 stays instead of the multiple $21^{p_i-1}2$. If there are two $p_i = 0$, then we have two cases: the sides of zero length are parallel or not. If $p_i = 0$ for three sides, then these sides pairwisely not parallel, and H degenerates into an equilateral triangle of sidelength p. If there are four i with $p_i = 0$, then the nonzero sides are opposite, H degenerates into a chain of $p_j + 1$ hexagons, and the sequence takes the form $41^{p_j-1}41^{p_j-1}$, where $p_j \geq 1$. If $p_i = 0$ for all i, we obtain an empty sequence corresponding to a hexagonal system consisting of one hexagon.

We prove below that, conversely, every hexagonal sequence without zeros has one of the above forms.

The equality (4) and Corollary 1 allow to enumerate all hexagonal sequences having no zeros.

Lemma 3 *A hexagonal sequence with $n_0 = 0$ has the following 7 possibilities for triples (n_2, n_3, n_4):*

n_2	0	0	3	0	2	4	6
n_3	0	1	0	3	2	1	0
n_4	2	1	1	0	0	0	0

Proof. If $n_0 = 0$, then from (4) and Corollary 1 we obtain

$$3n_4 + 2n_3 + n_2 = 6.$$

This equality implies $n_4 \leq 2$, $n_3 \leq 3$, $n_2 \leq 6$. An enumeration of all solutions of the equality gives the table of 7 solutions.

Call a sequence a by *S-sequence* if $a_i \in S$ for all i.

Note that we have no restriction on the number n_1 of ones in a hexagonal sequence. Hence hexagonal S-sequences $(1 \in S \subseteq \{1234\})$ have the form

$$a_1 1^{p_1} a_2 1^{p_2} ... a_m 1^{p_m}, \tag{12}$$

where $a_1 a_2 ... a_m$ is a pattern of a hexagonal S-$\{1\}$-sequence. Lemma 3 gives all (up to permutations) patterns of hexagonal S-sequences, $S \subseteq \{2, 3, 4\}$:

$$2^6,\ 2^4 3,\ 2^2 3^2,\ 3^3,\ 2^3 4,\ 34,\ 4^2. \tag{13}$$

It easy to verify by inspection that only the following patterns are themselves hexagonal sequences:

222222, 22223 , 2233, 2323 , 333, 44.

The condition $\lambda(a) = 6$ implies that the sequences 44 and 333 are the only sequences of length $l(a) = 2$ and 3.

Call a sequence a of length $k \geq 3$ *feasible* if the operation $f \equiv f_6$ can be applied to any triple of type $a3b$ and $a4b$ of a such that the obtained sequence again satisfies (3). It implies that a feasible sequence does not contain as a subsequence the triple $a4b$ with $a + b > 2$ and the pairs 34 and 43. Obviously, a hexagonal sequence is feasible.

For all S-sequences containing 4, we apply at first the operation f with respect to 4. As the proof of Proposition 1 below shows, such applications of f are sufficient to reduce the S-sequence with $S \ni 4$ either to 44 (and then the sequence is hexagonal) or to a non-feasible sequence.

Proposition 1 *All hexagonal (14)-sequences have the form* 41^p41^p *for* $p \geq 0$. *There are no hexagonal (134)- and (124)-sequences.*

Proof. We consider sequences with patterns 44, 34, 2^34. Begin with the sequence $41^{p_1}41^{p_2}$. If $p_1 = p_2 = 0$, we obtain the minimal sequence 44. If $p_1 > 0$, $p_2 = 0$, we obtain non-feasible sequence 441^{p_1}. Let $p_1 \geq p_2 \geq 1$. Then we have $41^{p_1}41^{p_2} \to 41^{p_1-1}41^{p_2-2}$ $\to 41^{p_1-p_2}4$. The last sequence is not feasible if $p_1 - p_2 > 0$.

For a (134)-sequence and $p_1 \geq p_2$, the reduction $31^{p_1}41^{p_2} \to 31^{p_1-p_2}4$ gives a non-feasible sequence. Similarly, any (124)-sequence $21^{p_1}21^{p_2}21^{p_3}41^{p_4}$ is reduced to a non-feasible sequence of type $21^{p_1}21^{p_2}21^q4$. The result follows.

For $S \subseteq \{123\}$, S-sequences satisfy the following property:

Lemma 4 *For* $S \subseteq \{123\}$, *an* S*-sequence has no two coinciding hexagons* h_i *and* $h_{i'}$ *with* $|i - j| \geq 2$.

Proof. If $h_i = h_{i'}$, then we can apply g^1_{ij} for $j = i' - 1$. Recall that the reduction $a \to g^{\pm 1}_{ij}(a)$ can be applied to a sequence a only if the inequalities (8) for $l = 1$ hold. For an S-sequence this means that $a_{i-1} = a_i = a_{j-1} = a_j = 1$. Let us apply g^1_{ij} to a sequence of type (12). Suppose at first that i and j belong to distinct strings of ones, say to 1^{p_1} and 1^{p_k}. Then

$$g^+_{ij}(a) = a_1 1^{p'_1-1}41^{p''_k-1}a_k...a_m1^m, \;\; g^-_{ij}(a) = 41^{p''_1-1}a_2...a_{k-1}1^{p'_k-1}.$$

Now apply f to $g^+_{ij}(a)$ and $g^-_{ij}(a)$ (with respect to 4) $\min(p'_1, p''_k) - 1$ and $\min(p''_1, p'_k) - 1$ times, respectively. We obtain non-feasible subsequences of type $x4y$ with $x + y > 2$. Similarly, it can be verified that applying g_{ij} with i and j from the same string of units gives non-feasible sequences. The result follows.

Lemma 4 shows that all hexagons h_i, $1 \leq i \leq k$, of an S-sequence a have connected intersections with C. It implies that we can apply the operation f to any h_i for a reduction of the sequence.

Now, for all patterns (13), using the operation f, we find hexagonal sequences without zeros. The last three cases are simplest. Recall that

$$f(x\hat{2}y) = x + 1, 0, y + 1, \;\; f(x\hat{3}y) = x + 1, y + 1 \;\; f(x\hat{4}y) = x + y + 2.$$

Denote as $a \to b$ that b can be obtained from a by applying operations f not increasing the length of a. We say that a is *reducible* to b. We use the following reductions (14) and (15).

$$x21^p2y \to x+1, 1^{p+1}, y+1. \quad (14)$$

This reduction is obtained as follows: $x\hat{2}1^p2y \to x+1, 0\hat{2}1^{p-1}2y \to x+1, 10\hat{2}1^{p-2}2y \to \ldots \to x+1, 1^{p-1}0\hat{2}2y \to x+1, 1^p0\hat{3}y \to x+1, 1^{p+1}, y+1$. Similarly, using $x2y \to x+1, 0, y+1$ and $x22y \to x+1, 03y \to x+1, 1, y+1$, we obtain the most important reduction

$$x2^py \to x+1, p-1, y+1. \quad (15)$$

We use this reduction for $p \geq 2$, when length of the sequence is decreased.

Note that the operation f closes in (14) and (15) hexagons of the sequences lying between x and y. It is easy to verify that two such hexagons h_i and h_j with $|i-j| \geq 2$ have no common edges.

For to find hexagonal sequences of other patterns, we have to consider at first the pattern 2^6. A hexagonal (12)-sequence has the form

$$a(p_1,p_2,p_3,p_4,p_5,p_6) = 21^{p_1}21^{p_2}21^{p_3}21^{p_4}21^{p_5}21^{p_6}$$

with $p_i \geq 0$, $1 \leq i \leq 6$.

Note that if $p_i = 0$ for some i in the notation $a(p_1,\ldots p_6)$, then the corresponding (1,2)-sequence has two consecutive 2's. Similarly, t consecutive zeros in $a(p_1,\ldots p_6)$ correspond to $t+1$ consecutive 2's.

Lemma 5 *A hexagonal (12)-sequence distinct from* $222222 = 2^6$ *contains at most 3 consecutive 2's.*

Proof. Let a (12)-sequence contains a subsequence $x12^p1y$, where $p \geq 4$ and $x, y = 1$ or 2. Then, by (15), $x12^p1y \to x2, p-1, 2y$. If $p > 5$, then $p-1 > 4$ and the sequence is not feasible. If $p = 5$, we obtain non-feasible sequence $x242y$, since $2+2 > 2$. If $p = 4$, we have $x232y \to x33y \to x+1, 4y$ with $x+1+y > 2$. The result follows.

Proposition 2 *All hexagonal (12)-sequences are* $a(p_1,p_2,p_3,p_4,p_5,p_6)$ *with non-negative* p_i *satisfying (11), or, equivalently, are as follows*

$$21^{p_1}21^{p-p_1-p_3}21^{p_3}21^{p-p_3-p_5}21^{p_5}21^{p-p_5-p_1},$$

where $p_1, p_3, p_5 \geq 0$, $p \geq p_i + p_j$, $ij = 13, 15, 35$. *In particular, the only hexagonal (12)-sequences with three pairs of consecutive 2's, with two triples of consecutive 2's and with six consecutive 2's are*

$221^p221^p221^p$, 2221^p2221^p *and* 222222,

when $p_1 = p_3 = p_5 = 0$; $p_3 = p_5 = 0$, $p = p_1$ *and* $p_1 = p_3 = p_5 = p = 0$, *respectively.*

Proof. Consider the sequence $a(p_1,p_2,p_3,p_4,p_5,p_6) = 21^{p_1}21^{p_2}21^{p_3}21^{p_4}21^{p_5}21^{p_6}$ at first with $p_i > 0$, $1 \leq i \leq 6$. Applying (14) to 21^x2 for $x = p_2, p_5$ we obtain $a(p_1,\ldots,p_6) \to$

$a(p_1-1,p_2+1,p_3-1,p_4-1,p_5+1,p_6-1)$. Let $p=\min(p_1,p_3)$, $p'=\min(p_4,p_6)$. Applying (14) p and p' times, we obtain $a(p_1,...,p_6)\to a(p_1-p,p_2+p,p_3-p,p_4-p',p_5+p,p_6-p')$.

We have the following cases: $p_1=p<p_3$, $p_1=p=p_3$, $p_1>p=p_3$ and $p_4=p'<p_6$, $p_4=p'=p_6$, $p_4>p'=p_6$. There are 9 the following combinations:

1.	$p_1=p<p_3,$	$p_4=p'<p_6$	$a(0,p_2+p_1,p_3-p_1,0,p_5+p_4,p_6-p_4)$		$\alpha)$
2.	$p_1=p<p_3,$	$p_4=p'=p_6$	$a(0,p_2+p_1,p_3-p_1,0,p_5+p_4,0)$	$p_4=p_6$	$\gamma)$
3.	$p_1=p<p_3,$	$p_4>p'=p_6$	$a(0,p_2+p_1,p_3-p_1,p_4-p_6,p_5+p_6,0)$		$\beta)$
4.	$p_1=p=p_3,$	$p_4=p'<p_6$	$a(0,p_2+p_1,0,0,p_5+p_4,p_6-p_4)$	$p_1=p_3$	$\gamma)$
5.	$p_1=p=p_3,$	$p_4=p'=p_6$	$a(0,p_2+p_1,0,0,p_5+p_4,0)$ $\quad p_1=p_3,$	$p_4=p_6$	$\delta)$
6.	$p_1=p=p_3,$	$p_4>p'=p_6$	$a(0,p_2+p_1,0,p_4-p_6,p_5+p_6,0)$	$p_1=p_3$	$\gamma)$
7.	$p_1>p=p_3,$	$p_4=p'<p_6$	$a(p_1-p_3,p_2+p_3,0,0,p_5+p_4,p_6-p_4)$		$\beta)$
8.	$p_1>p=p_3,$	$p_4=p'=p_6$	$a(p_1-p_3,p_2+p_3,0,0,p_5+p_4,0)$	$p_4=p_6$	$\gamma)$
9.	$p_1>p=p_3,$	$p_4>p'=p_6$	$a(p_1-p_3,p_2+p_3,0,p_4-p_6,p_5+p_6,0)$		$\alpha)$

Up to symmetry and cyclic shift these 9 cases give (12)-sequences of the following 4 types:

$\alpha)$ $a(0,q_2,q_3,0,q_5,q_6)=221^{q_2}21^{q_3}221^{q_5}21^{q_6}$

$\beta)$ $a(0,0,q_3,q_4,q_5,q_6)=2221^{q_3}21^{q_4}21^{q_5}21^{q_6}$

$\gamma)$ $a(0,0,q_3,q_4,0,q_6)=2221^{q_3}21^{q_4}221^{q_6}$

$\delta)$ $a(0,0,q_3,0,0,q_6)=2221^{q_3}2221^{q_6}$

For example, in the sequence of type $\alpha)$, for cases 1 and 9, we have, respectively,

$$q_2=p_2+p_1,\ q_3=p_3-p_1,\ q_5=p_5+p_4,\ q_6=p_6-p_4$$

$$q_2=p_1-p_3,\ q_3=p_2+p_3,\ q_5=p_4-p_6,\ q_6=p_5+p_6.$$

Now we consider the cases when $p_i=0$ for some i and we cannot apply (14) as above. If there is only one such i, then we can suppose that $i\neq 2,5$, and then either $p=0$ or $p'=0$, and we apply (14) for p or p' not equal to zero. If there are exactly two i with $p_i=0$, then we have either one of the cases $\alpha)$ or $\beta)$, or $a(0,q_2,0,q_4,q_5,q_6)$. But the last case is obtained from $a(p_1,...,p_6)$ applying (14) to $21^{p_2}2$ when $p_1=p_3$. Hence it gives one of cases 4, 5 or 6.

So, the cases $\alpha)$-$\delta)$ cover also all possible cases of $a(p_1,...,p_6)$ with $p_i=0$ for some i. Let us now to apply (14) to $21^{q_2}2$ of the sequence of type $\alpha)$. We have

$221^{q_2}21^{q_3}221^{q_5}21^{q_6}\to 31^{q_2+1}21^{q_3-1}221^{q_5}21^{q_6}\to 221^{q_2}21^{q_3-1}221^{q_5}21^{q_6-1}$.

Let $q=\min(q_3,q_6)$. Up to symmetry, we have two cases: $q=q_3=q_6$ and $q=q_3<q_6$. Applying q times (14) to $\alpha)$ we obtain in these two cases $a(0,q_2,q_3,0,q_5,q_6)\to a(0,q_2,0,0,q_5,0)$ and $a(0,q_2,q_3,0,q_5,q_6)\to a(0,q_2,0,0,q_5,q_6-q)$, i.e. the sequences of types $\delta)$ and $\gamma)$, respectively. Hence we can consider only sequences of types $\beta)$, $\gamma)$, $\delta)$.

Now we apply (15) to the first three 2's of the sequence of type $\beta)$ and get

$a(0,0,q_3,q_4,q_5,q_6)\to a(0,0,q_3-1,q_4,q_5,q_6-1)$.

Setting $q=\min(q_3,q_6)$, we have two cases $q=q_3=q_6$ and $q=q_3<q_6$. Applying q times (15), we obtain $a(0,0,q_3,q_4,q_5,q_6)\to$ either $a(0,0,0,q_4,q_5,0)=2^51^{q_4}21^{q_5}$ or $a(0,0,0,q_4,q_5,q_6-q)=2^41^{q_4}21^{q_5}21^{q_6-q}$. By Lemma 5, both these sequences are not hexagonal.

Similarly, we obtain that the sequence of type γ) is not feasible. For sequences of type δ), using (15), we obtain $2^3 1^{s_1} 2^3 1^{s_2} \to 2^3 1^{s_1-1} 2^3 1^{s_2-1} \to 2^6 1^{s_1-s_2}$, where we suppose w.l.o.g. that $s_1 \geq s_2$. By Lemma 5, this sequence is hexagonal only if $s_1 = s_2$.

Now remember what are the values of s_1 and s_2 in a sequence of type δ). If the sequence is obtained from a sequence of type α), then

$s_1 = q_2 = p_2 + p_1$, $s_2 = q_5 = p_5 + p_4$, $q_3 = p_3 - p_1$, $q_6 = p_6 - p_4$ in case 1,

$s_1 = q_2 = p_1 - p_3$, $q_3 = p_2 + p_3$, $s_3 = q_5 = p_4 - p_6$, $q_6 = p_5 + p_6$ in case 9,

and $q_3 = q_6$ in both these cases.

In case 5 we have $s_1 = p_1 + p_2$, $s_2 = p_4 + p_5$ and $p_1 = p_3$, $p_4 = p_6$. The equalities $s_1 = s_2$ and $q_3 = q_6$ imply that $p_1 - p_4 = p_5 - p_2 = p_3 - p_6 = q$ for all these cases. Setting $p = p_1 + p_3 + p_5 - q$, we obtain the assertion of the proposition.

So, it remains to consider the patterns 333, $2^2 3^2$ and $2^4 3$.

Proposition 3 *(i) All hexagonal (13)-sequences have the form* $31^p 31^p 31^p$ *for* $p \geq 0$.

(ii) All hexagonal (123)-sequences have the form $31^p 21^q 31^p 21^q$, $21^p 31^{p+q+1} 31^p 21^q$, $21^p 21^{q+r+1} 31^{p+r+1} 21^q 21^r$ *for* $p, q, r \geq 0$.

Proof. (i) Consider a (13)-sequence $31^{p_1} 31^{p_2} 31^{p_3}$. Suppose at first that $p_i \geq 2$ for all i. Then using the reduction $131 \to 22$, we obtain $31^{p_1} 31^{p_2} 31^{p_3} \to 221^{p_1-2} 221^{p_2-2} 221^{p_3-2}$. By Proposition 2, such a sequence is hexagonal only if $p_1 = p_2 = p_3$. Now let $p_1 = 0$ and $p_2, p_3 \neq 0$. Then we obtain a non-feasible sequence: $1331 \to 241 \to 5$. Similarly, we find that the case $p_1 = p_2 = 0$ and $p_3 \neq 0$ is not hexagonal. Now if $p_1 = 1$, $p_2 = 1$, $p_3 > 1$, we obtain a non-feasible sequence: $31\hat{3}1311 \to 322\hat{3}11 \to 32\hat{3}21 \to 3\hat{3}31 \to 441$. Similarly, if $p_1 = 1$, $p_2, p_3 > 1$, we obtain a non-feasible sequence.

(ii) There are three (23)-patterns: a) 3232, b) 2332 and c) 22322. We set

$$a(p_1, p_2; p_3, p_4) = 31^{p_1} 21^{p_2} 31^{p_3} 21^{p_4} \sim a(p_2, p_1; p_4, p_3) \sim a(p_3, p_4; p_1, p_2),$$

$$b(p_1, p_2, p_3, p_4) = 21^{p_1} 31^{p_2} 31^{p_3} 21^{p_4} \sim b(p_3, p_2, p_1, p_4),$$

$$c(p_1, p_2; p_3, p_4; p_5) = 21^{p_1} 21^{p_2} 31^{p_3} 21^{p_4} 21^{p_5} \sim c(p_4, p_3; p_2, p_1; p_5).$$

Consider at first $c(p_1, p_2; p_3, p_4; p_5)$. If $p_2, p_3 > 0$, then we apply the reduction $131 \to 22$ that gives $c(p_1, p_2; p_3, p_4; p_5) \to 21^{p_1} 21^{p_2-1} 221^{p_3-1} 21^{p_4} 21^{p_5} \sim 21^{p_2-1} 221^{p_3-1} 21^{p_4} 21^{p_5} 21^{p_1}$. Now we apply Proposition 2, where we denote p_i, p by q_i, q. We use the shift of our sequence, since $q_2 = q_5 - q \leq q_5$ in the sequence of Proposition 2. Comparing we obtain: $q_1 = p_2 - 1$, $q_5 - q = 0$, $q_3 = p_3 - 1$, $q_1 - q = p_4$, $q_5 = p_5$, $q_3 - q = p_1$. From these equalities we obtain the following dependencies between p_i:

$$p_2 = p_4 + p_5 + 1, \; p_3 = p_1 + p_5 + 1. \tag{16}$$

Note that these equalities imply $p_2, p_3 > 0$. Hence if $p_2, p_3 > 0$, then $c(p_1, p_2; p_3, p_4; p_5)$ is hexagonal if and only if the equalities (16) hold.

Suppose that $p_2 = 0$. Then we have the subsequence $zx23yt$, where $x = 2$ if $p_1 = 0$, $x = 1$ if $p_1 > 0$, $y = 2$ if $p_3 = 0$, $y = 1$ if $p_3 > 0$, and $z, t \geq 1$. Consider the reductions:

$$zx23yt \to zx3, y+1, t \to z, x+1, y+2, t.$$

If $p_3 = 0$, then $y + 2 = 4$, and we obtain a non-feasible sequence, since $x+1, 4t \to x+t+3 \geq 5$. Hence $c(p_1, 0; 0, p_4; p_5)$ is not hexagonal. If $p_3 > 0$, then $y+2 = 3$, and we have $z, x+1, 3, t \to z, x+2, t+1$. If $p_1 = 0$, then $x+2 = 4$, and we have $z4, t+1 \to z+t+3 \geq 5$, and again we obtain a non-feasible sequence. Hence the sequences $c(0, 0; p_3, p_4; p_5) \sim c(p_4, p_3; 0, 0; p_5)$ are not hexagonal. If $p_1 > 0$, (and $p_3 > 0$) then we have the reduction $c(p_1, 0; p_3, p_4; p_5) \to c(p_1 - 1, 0; p_3 - 1, p_4; p_5)$. Let $p = \min(p_1, p_3)$. We apply this reduction p times. In both the cases $p = p_1$ or $p = p_3$, we obtain non-hexagonal sequences $c(0, 0; p_3 - p_1, p_4; p_5)$ or $c(p_1 - p_3, 0; 0, p_4; p_5)$. So, we obtain that

$c(p_1, p_2; p_3, p_4; p_5)$ is hexagonal if and only if $p_2, p_3 > 0$ and the equalities (16) hold.

If $p_1, p_4 > 0$, then $a(p_1, p_2; p_3, p_4) \to 21^{p_1-1}21^{p_2}31^{p_3}21^{p_4-1}2 = c(p_1 - 1, p_2; p_3, p_4 - 1; 0)$, which is hexagonal only if $p_2, p_3 > 0$. Hence the sequences $a(p_1, 0; p_3, p_4) \sim a(0, p_1; p_4, p_3) \sim a(p_3, p_4; p_1, 0) \sim a(p_4, p_3; 0, p_1)$ are not hexagonal for $p_1, p_4 > 0$, $p_3 \geq 0$. If both $p_2, p_3 > 0$, then the equalities (16) imply $p_2 = p_4$, $p_3 = p_1$. Hence if $p_i > 0$ for all i, then

$$a(p_1, p_2; p_3, p_4) \text{ is hexagonal if and only if } p_1 = p_3,\ p_2 = p_4. \tag{17}$$

It is easy to verify that $a(0, p_2; 0, p_4) \to a(p_2 - 1, 0; p_4 - 1, 0) \sim a(0, p_2 - 1; 0, p_4 - 1)$. Continuing, we see that $a(0, p_2; 0, p_4)$ is hexagonal only if $p_2 = p_4$. By symmetry, we obtain that (17) is true for $p_i \geq 0$, $1 \leq i \leq 4$.

As above, we obtain that if $p_1, p_2 > 0$, then $b(p_1, p_2, p_3, p_4) \to 21^{p_1-1}221^{p_2-1}31^{p_3}21^{p_4} = c(0, p_2 - 1; p_3, p_4; p_1 - 1)$. This sequence is hexagonal if and only if $p_2 > 1$, $p_3 > 0$. If $p_2 > 1$, $p_3 > 0$ the equalities (16) imply $p_2 = p_1 + p_4 + 1$, $p_3 = p_1$. Hence if $p_1 > 0$

$$b(p_1, p_2, p_3, p_4) \text{ is hexagonal if and only if } p_2 = p_1 + p_4 + 1,\ p_3 = p_1. \tag{18}$$

Let $p_1 = 0$. Then

$$b(0, p_2, p_3, p_4) \to a(0, p_2 - 1, p_3, p_4),$$

which is, by (17), hexagonal if and only if $p_3 = 0$ and $p_2 = p_4 + 1$. Hence (18) holds for $p_1, p_4 \geq 0$. The result follows.

Proposition 4 *A hexagonal sequence a without zeros determines unique partition of the disc $D(a)$ into hexagons.*

Proof. Note that the hexagons h_i adjacent to $C(a)$ with $a_i \geq 3$ are uniquely determined by a in any partition determined by a. It is easy to see that operations f with respect to $a_i = 3$, (14) and (15) transform a hexagonal sequence without zeros into another hexagonal sequence without zeros of less length. Besides (14) as well as (15) applied to distinct strings commute. Now, by induction, the result follows.

This proposition induces the following

Problem. *Is it true that any hexagonal sequence a determines uniquely the partition of $D(a)$ into hexagons?*

It is proved in [CaHa98] that the answer is "yes" if the hexagonal sequence a corresponds to a hexagonal system that can be embedded into the hexagonal lattice of regular hexagons. We are thankful to Gunnar Brinkmann for informing us about results of work [CaHa98].

5 One-pent hexagonal sequences without zeros

Consider now convex sequences corresponding to partitions containing one pentagon. Following to [BDPS97], call such a sequence *one-pent hexagonal.* By (5), $\lambda(a) = 5$ and the equality (4) takes the form

$$3n_4 + 2n_3 + n_2 = 5.$$

This equation gives the following possibilities for n_i:

n_2	0	2	1	3	5
n_3	1	0	2	1	0
n_4	1	1	0	0	0

Now, besides the operation $f = f_6$, we have to apply exactly one time the operation f_5. In this case, the minimal non-empty sequence is 34. It corresponds to a pentagon adjacent to a hexagon. Recall that f_5 cannot be applied with respect to 4, and

$$f_5(x\hat{1}y) = x+1, 0, y+1, \ \ f_5(x\hat{2}y) = x+1, y+1 \ \ f_5(x\hat{3}y) = x+y+2.$$

Clearly, after an application f_5 to a one-pent hexagonal sequence, the obtained sequence should be hexagonal. Hence it is easy to prove the following assertions.

Proposition 5 *(i) All one-pent hexagonal (134)-sequences have the form* 31^p41^p, $p \geq 4$.

(ii) There are no one-pent hexagonal (124)-sequences.

(iii) An application f_5 to a one-pent hexagonal (123)-sequence with respect to 3 gives a non-hexagonal sequence.

Similarly, as it was done for hexagonal sequences, we set

$$a(q_1, q_2, q_3, q_4, q_5) = 21^{q_1}21^{q_2}21^{q_3}21^{q_4}21^{q_5}.$$

We set also

$$c(q) = 21^q221^{q+1}3 \cong 221^q31^{q+1}.$$

It is not difficult to verify that the sequence $c(q)$ is one-pent hexagonal for all $q \geq 0$.

Using (ii) and (iii) of Proposition 5, we obtain the following for (123)-sequences of shape 2^33.

Proposition 6 *For a one-pent hexagonal sequence of the form* $21^{q_1}21^{q_2}21^{q_3}31^{q_4}$ *we have:*

(i) The condition $q_4 = 0$ *implies* $q_2 = 0$, $q_3 = q_1 + 1 = q + 1$, *and the condition* $q_3 = 0$ *implies* $q_1 = 0$, $q_4 = q_2 + 1 = q + 1$. *Both these cases give one-pent hexagonal sequences of type* $c(q)$.

(ii) If $q_4 > 0$ *and* $q_3 > 0$, *then* $21^{q_1}21^{q_2}21^{q_3}31^{q_4} \to a(q_1, q_2, q_3 - 1, 0, q_4 - 1)$.

Now we consider the shape 23^2.

Proposition 7 *For a one-pent hexagonal sequence of the form* $21^{q_1}31^{q_2}31^{q_3}$ *we have:*

(i) The condition $q_2 = 0$ *implies* $q_1 = q_3 = 0$, *and we obtain the one-pent hexagonal sequence 233.*

(ii) The condition $q_2 = 1$ *implies* $q_1 = q_3 = 1$, *and we obtain the one-pent hexagonal sequence 213131*$\to c(0)$.

(iii) If $q_2 = q \geq 2$, *then* $q_1 = 0$ *implies* $q_3 = q$, *and* $q_3 = 0$ *implies* $q_1 = q$. *Both these cases are reduced to* $c(q - 2)$.

(iv) If $q_2 \geq 2$, $q_1 \geq 1$, $q_3 \geq 0$, *then* $21^{q_1}31^{q_2}31^{q_3} \to a(q_1 - 1, 0, q_2 - 1, 0, q_3 - 1)$.

For to find *all* one-pent hexagonal (123)-sequences, we have to determine all (12)-sequences. But the last problem is difficult enough. We know only a partial answer. It is easy to identify all sequences corresponding to partitions, where the pentagon has a common edge with the boundary.

Proposition 8 *There are the following one-pent hexagonal (12)-sequences:*

$a(p + q, q + r + 1, p, q, r)$ *if the pentagon touches the boundary by two edges that relate to* $a_{p+q+2} = 1$;

$a(p + q + 1, q + r + 1, p, q, r)$ *if the pentagon touches the boundary by three edges that relate to* $a_{p+q+2} = 2$;

$a(p + q, q + r, p, q, r)$ *if the pentagon is separated from the boundary by a hexagon; here* p, q, r *are non-negative integers.*

Additionally, we have the following lemma.

Lemma 6 *If* $a(q_1, q_2, q_3, q_4, q_5)$ *is a one-pent hexagonal (12)-sequence, then so is* $a(q_1 + s, q_2 + s, q_3 + s, q_4 + s, q_5 + s)$ *for* $s \geq 0$. *In particular, the sequence* $21^p21^p21^p21^p21^p$ *is one-pent hexagonal for all non-negative integers* p.

Proof. We can add a ring R of hexagon in the outer domain $\overline{D}(a)$ of the circuit $C(a)$. Then the outer circuit of R determines the sequence $(\overline{a})^*$. Using the definition of the complementary sequence $\overline{a}$, given in Section 2, we have

$$(\overline{a(q_1, ..., q_5)})^* = (\overline{21^{q_1}2...21^{q_5}})^* = (01^{q_1+1}01^{q_2+1}01^{q_3+1}01^{q_4+1}01^{q_5+1})^* = 21^{q_1+1}2...21^{q_5+1}.$$

Obviously, if a is one-pent hexagonal, then so is $(\overline{a})^*$. The result follows.

Remark. For a hexagonal sequence the above assertion holds with "if and only if". This is not true for one-pent hexagonal sequences, what show sequences with a pentagon touching the boundary.

6 Hexagonal sequences of small length

For to find hexagonal sequences of length $k \geq 4$, we define the reciprocal operation f^*. For $a \geq 1$, $b \geq 1$, we set

$$f^*(a0b) = a-1, 2, b-1, \ f^*(ab) = a-1, 3, b-1.$$

For $c \geq 2$, we define 3 operations f^*, f'^*, f''^*.

$f^*(c) = c-4, 4, 2 = 042$ or $f^*(c) = 2, 4, c-4 = 240$ if $c = 4$,

$f'^*(c) = c-3, 4, 1$ or $f'^*(c) = 1, 4, c-3$ if $c \geq 3$,

$f''^*(c) = c-2, 4, 0$ or $f''^*(c) = 0, 4, c-2$ if $c \geq 2$.

So, we have the following transformations

4⇒ 042, 240, 141; 3⇒ 041, 140; 2⇒ 040.

The operation $f^*(a0b)$ does not change and $f^*(ab)$ increases by 1 the length of a sequence. All the operations $f^{(i)*}(c)$ increase the length of a sequence by 2. Hence, for to obtain a hexagonal sequence of length 3 from the sequence 44, we apply the first operation $f^*(44) = 333$.

Applying the first operation to 333, we obtain the sequence 2323. From this sequence, using the operation f, we obtain

$f(\hat{2}323) = 0424 = (f^*(4)4) = 4f''^*(4)$.

Besides, we have $f'^*(4)4$=1414.

Applying the operations f^* to sequences of length $k-1$ and $k-2$, we obtain sequences of length k. All hexagonal sequences of length k, $2 \leq k \leq 7$, are given in Table 1.

Table 1. Hexagonal sequences of length at most 7.

k	$h(a)$	hexagonal sequences			
2	2	44			
3	3	333			
4	4	2323			
	3	0424	1414		
5	5	23132			
	4	04133			
6	7	222222			
	6	032223		123123	131313
	5	040323	033033	204123	
	4	040404	042240	014124	204204
	4	114114			
7	8	2213122			
	7	3023122	0313123		1321231
	6	3104122	3023203	0313204	1402231
	5	3104203	4104130	1410331	1403041
	5	0033124	0413140		

Recall that we can obtain a sequence of length k from another sequence a of length k if a contains $a_i = 2$ and we can apply the operation f to the triple $a_{i-1}2a_{i+1}$. Of course,

$h(f(a)) = h(a) - 1$. Hence, for given k, we set in Table 1 the sequence $f(a)$ below the sequence a, or below and right, (and, for $k = 7$, below, below and right, below and left) if there are two or more sequences $f(a)$, i.e. when a has $a_i = 2$ for two or more i.

But not all hexagonal sequences of length k can be obtained from sequences of length $k-1$ and $k-2$ by operations f^*. For example, there are irreducible sequences that cannot be obtained from sequences of smaller length.

7 Fullerenes with an isolated ring of hexagons

In [DeGr97b], $6R_2$-*fullerenes* 5_n are considered such that each its hexagon is adjacent exactly to two other hexagons. Hence the hexagons of such fullerenes form rings of hexagons of length $k \geq 3$. If $k = 3$, the ring degenerates into a triple of mutually adjacent hexagons.

Suppose that a $6R_2$-fullerene has a ring R of hexagons of length $k \geq 4$ such that the inner domain $D(R)$ of the ring R is partitioned into only pentagons. This means that the inner boundary circuit C of R is the boundary circuit of $D(R)$. As above, we relate to C a sequence $a_1 a_2 ... a_k$, whose tails correspond to edges by which the hexagons of R are adjacent to each other. It implies that the sequence $a_1 ... a_k$ is irreducible.

So, the problem is to find configurations of pentagons such that the boundary of any configuration generates an irreducible sequence.

We proceed as follows. Suppose we have a configuration of p pentagons the boundary of which gives a sequence $a = a_1 ... a_q$. For to obtain a configuration of $p+1$ pentagons, we connect two neighboring tails t_i and t_{i+1} such that they form a pentagon, i.e. we apply the operation f_p for $p = 5$ (see (7)).

If the sequence a has an element $a_i = 4$, then the tails t_i and t_{i+1} cannot form a pentagon.

Beginning with the sequence 00000 corresponding to the boundary of a pentagon, we form sequences corresponding to the boundaries of configurations of s pentagons. For $s \leq 6$, we obtain the sequences given in Table 2. (note that the tails of the sequences lie outside the domain filled by pentagons.)

Table 2. Pentagonal sequences of length at most 6

$s = 1$	00000				
$s = 2$	010010				
$s = 3$	010101	1002001			
$s = 4$	101101	0102002	20012001	11003001	
$s = 5$	020111 100400111	2101200 121002200	00301021	00300202	001300112
$s = 6$	11111 22002200 001300203 1002300112	020202 10301030 003003003 0013100212	021021 004010211 0014001112 0012200122	0030112 004002021 100500111	10130012 001301022 0011300113

Similarly, as it was done for a ring of hexagons, we can define a duality a^+ of a sequence a using a ring of pentagons. A sequence $a_1 ... a_k$ defines a ring of pentagons only if $0 \leq a_i \leq 1$ for all i. We call such a sequence *π-irreducible*. For a π-irreducible sequence a, $a_i^+ = 1 - a_i$.

We try to construct all $6R_2$-fullerenes having a ring R of hexagons of length $k \geq 4$. Recall that every fullerene contains exactly 12 pentagons. Let the inner domain of R contains s pentagons.

If $s = 1$, the pentagon is surrounded by a ring R_1 of 5 hexagons. The ring R_1 transforms the sequence 00000 into the sequence $\overline{(00000)^*} = \overline{22222}$=0101010101. We obtain a sequence of length 10, i.e. the ring R_1 is surrounded by at least 10 pentagons. Since the sequence 0101010101 π-is irreducible, there exists a ring of 10 pentagons. This ring of pentagons transforms the sequence 0101010101 into the sequence $\overline{(0101010101)^+} = \overline{1010101010}$=22222. Now a new ring of 5 hexagons transforms 22222 into $(22222)^*$=00000, but the last sequence 00000 corresponds to a pentagon.

So, we obtain a $6R_2$-fullerene with two rings of hexagons, each containing 5 hexagons. Since this fullerene contains $\frac{1}{3}(10 \times 6 + 12 \times 5) = 40$ vertices, we obtain $5_{40}(D_{5h})$. Here and below we give in parentheses the group of symmetry of the corresponding fullerene.

If $s = 2$, we have the sequence 010010 of length 6. Hence the two pentagons are surrounded by a ring R_2 of 6 hexagons. R_2 transforms 010010 into the sequence $\overline{(010010)^*} = \overline{212212}$ = 0110101101 of length 10. Hence R_2 is surrounded by at least 10 pentagons, i.e. by exactly 10 pentagons. This ring of pentagons transforms 0110101101 into $\overline{(0110101101)^+} = \overline{1001010010} = 3232$. Since we have used all 12 pentagons, this sequence should be hexagonal. As we see from Table 1, it is hexagonal indeed and it defines a partition of the outer domain of the ring of 10 pentagons into 4 hexagons. We obtain another fullerene $5_{40}(C_2)$, but it is not $6R_2$.

For $s = 3$, we have two sequences, both irreducible. The sequence 010101 defines a ring R_3 of 6 hexagons. R_3 transforms 010101 into the sequence $\overline{(010101)^*} = \overline{212121}$ = 011011011 of length 9. Hence R_3 is surrounded by a ring of 9 pentagons. This ring transforms 011011011 into $\overline{(011011011)^+} = \overline{100100100} = 333$. This last sequence is hexagonal and defines a partition of the outer domain of the ring of 9 pentagons into 3 hexagons. We obtain a fullerene $5_{38}(C_{3v})$.

The second sequence 1002001 defines a ring R_3' of 7 hexagons. R_3' transforms 1002001 into the sequence 0102010111 of length 10. Hence R_3' should be surrounded by at least 10 pentagons. Since a fullerene has 12 pentagons, we see that the configuration of 3 pentagons with the sequence 1002001 does not define a fullerene.

For $s = 4$, we have 3 irreducible sequences. The sequence 101101 defines a ring R_4 of 6 hexagons. R_4 transforms 101101 into the sequence 01110111 of length 8, which is π-irreducible. Hence R_4 is surrounded by a ring of 8 pentagons. This ring of pentagons transforms 01110111 into the hexagonal sequence 44. We obtain a fullerene 5_{36} with 8 hexagons which is not $6R_2$. As in the case $s = 3$, we find that the sequences 0102002 and 20012001 do not define fullerenes.

For $s = 5$, we have 3 irreducible sequences. For the first sequence 020111 we have $\overline{(020111)^*}$ = 2011110. This sequence is not π-irreducible, but the 7 pentagons surrounding the ring of 5 hexagons have as the outer domain a hexagon. So, we obtain a fullerene 5_{32}, which is not $6R_2$. As above, we can show that the other two sequences of length 7 and 9 do not define fullerenes.

For $s = 6$, we obtain the following 5 irreducible sequences:
11111, 020202, 021021, 22002200, 0012200122.

Note that these sequences are self-dual. Hence they define 5 fullerenes with a ring of hexagons of length k=5, 6, 6, 8, 10, respectively. Since the sequences are self-dual, the partitions into pentagons of the outer domain and the inner one are similar, each containing 6 pentagons. Since a fullerene has exactly 12 pentagons, we obtain that the 12 pentagons and k hexagons are all faces of these fullerenes, which are:

$5_{30}(D_{5h})$, $5_{32}(D_{3d})$, $5_{32}(D_{2h})$, $5_{36}(D_{2d})$, $5_{40}(D_2)$,
in the order corresponding to the order of above 5 sequences.

8 Fullerenes with the ring of 12 pentagons

This is case (5) of $5R_2$ fullerenes from Section 3 of [DeGr97b].

The simplest example applying of hexagonal sequences is related to fullerenes 5_n, where the 12 pentagons form a ring. We represent the ring of pentagons as a ring of 12 quadrangles. Each of the inner C^i and outer C^o boundary circuits contains 12 vertices. We have to set between these 12 vertices k tails on edges of C^i and l tails on edges of C^o, by one in each quadrangle, for to obtain pentagons from the quadrangles. After that we obtain two sequences $a = a_1...a_k$ and $b = b_1...b_l$, where $k+l = 12$, and $\sum_1^k a_i = \sum_1^l b_i = 12$. For to obtain a fullerene, these sequences should be hexagonal, i.e. should be $\lambda(a) = \lambda(b) = 6$. The equation (1) implies $k = l = 6$. Besides, by construction, we have $a_i \geq 1$, $b_i \geq 1$, and the sequences a and b should be consistent in the following sense. We relate to the sequence a a sequence $\tilde{a}$ of zeros and ones such that a_i is transformed into 10...0 with $a_i - 1$ zeros. We obtain $\tilde{a}$ and $\tilde{b}$. In our case, both $\tilde{a}$ and $\tilde{b}$ have length 12, the number of quadrangles in the ring. 1's of the sequences $\tilde{a}$ and $\tilde{b}$ show in which quadrangles the tails were set. Hence $\tilde{a} + \tilde{b} = \tilde{1}$, where $\tilde{1}$ denotes all ones sequence, and the addition is component-wise.

Among hexagonal sequences of length 6, there are only the following 4 sequences with all $a_i \geq 1$:

$a^1 = 222222$, $a^2 = 123123$, $a^3 = 131313$, $a^4 = 114114$.

We have

$$\tilde{a}^1 = 101010101010, \tilde{a}^2 = 110100110100, \tilde{a}^3 = 110011001100, \tilde{a}^4 = 111000111000.$$

We see that $1 - \tilde{a}^i$ is a shift of the same sequence $\tilde{a}^i$ for all these sequences. This means that there are only four fullerenes with a ring of 12 pentagons. Each of these fullerenes has similar hexagonal partitions in the outer and inner domains of the ring. Drawings of these partitions are given on Fig.6 of [DeGr97a].

9 Fullerenes with two rings by 6 pentagons

This is case (4) of $5R_2$ fullerenes from Section 3 of [DeGr97b].

Now we consider the case when a fullerene has two 6-cycles of pentagons. Consider, as in previous section, two rings R_1 and R_2 of 6 quadrangles. We have to set 6 tails on edges of the outer and the inner boundary of R_1. Suppose that the second ring R_2 lies in the outer domain of R_1. Then the inner boundary of R_1 should give a hexagonal sequence $a_1 ... a_k$ such that $\sum_1^k a_i = 6$, the number of quadrangles in R_1. Using (5), we see that $k = 0$, i.e. the inner domain of R_1 consists of a unique hexagon. Similarly, the inner domain of R_2 is also a hexagon.

Hence all tails are in the outer domains of R_1 and R_2, and we have two equal Petrie sequences 111111 of length 6, corresponding to the outer boundaries of R_1 and R_2. Recall that a Petrie sequence is self-dual and irreducible. Our sequence of length 6 uniquely determines a ring of 6 hexagons. Consider the ring R_1 surrounded by such a ring R_0 of 6 hexagons. The boundary of R_0 determines the sequence $(111111)^*$=111111. So we come to a situation similar to the original one. This implies that fullerenes with two 6-cycles of pentagons consist of those cycles of pentagons separated by a number of rings each containing 6 hexagons.

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